

di-(3-Methoxybutyl)sebacate

Inchi:	InChI=1S/C20H38O6/c1-17(23-3)13-15-25-19(21)11-9-7-5-6-8-10-12-20(22)26-16-14-18
InchiKey:	VBNBOVAVLMAHMM-UHFFFAOYSA-N
Formula:	C20H38O6
SMILES:	COC(C)CCOC(=O)CCCCCCCCC(=O)OCCC(C)OC
Mol. weight [g/mol]:	374.51

Physical Properties

Property code	Value	Unit	Source
gf	-565.20	kJ/mol	Joback Method
hf	-1220.73	kJ/mol	Joback Method
hfus	48.46	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.044		Crippen Method
mcvol	319.280	ml/mol	McGowan Method
pc	1065.18	kPa	Joback Method
rinpol	2447.00		NIST Webbook
rinpol	2447.00		NIST Webbook
tb	853.54	K	Joback Method
tc	1045.67	K	Joback Method
tf	473.94	K	Joback Method
vc	1.228	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.21	J/molxK	853.54	Joback Method
cpg	1051.02	J/molxK	885.56	Joback Method
cpg	1067.56	J/molxK	917.58	Joback Method
cpg	1082.82	J/molxK	949.60	Joback Method
cpg	1096.81	J/molxK	981.62	Joback Method
cpg	1109.52	J/molxK	1013.65	Joback Method
cpg	1120.96	J/molxK	1045.67	Joback Method
dvisc	0.0005246	Paxs	473.94	Joback Method

dvisc	0.0002339	Paxs	537.21	Joback Method
dvisc	0.0001237	Paxs	600.47	Joback Method
dvisc	0.0000738	Paxs	663.74	Joback Method
dvisc	0.0000482	Paxs	727.01	Joback Method
dvisc	0.0000337	Paxs	790.27	Joback Method
dvisc	0.0000248	Paxs	853.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542268&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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